



Two-Dimensional Simulation of Diffusion and Advection Effects in Enzymatic Hydrolysis of Cellulose

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Abstract. Enzymatic hydrolysis process to transform lignocellulosic cellulose into sugar in a bioreactor tank involves different controlling factors such as advection, diffusion and fragmentation of cellulose chains. Although it has been observed experimentally that enzymatic hydrolysis is strongly influenced by the environmental effects in a tank, these effects have not been adequately quantified. In this work, a current kinetic model for enzymatic hydrolysis of cellulose was extended by coupling the *population balance equations* (PBE) with advection and diffusion terms to model the spatial evolution of the system. The mathematical model was solved using the DAE-QMOM technique. The aim of this study was to simulate the effect of diffusion and advection on the fragmentation of cellulose chains during enzymatic hydrolysis in two-dimensional domain. This study demonstrated the applicability and usefulness of a commercial software (*COMSOL Multiphysics*) for finding the solution of PBE-advection-diffusion in cellulosic hydrolysis problem. The key implication of this work is that advection is a significant phenomenon which could increase the number of cellulose particles. Also, diffusion alone cannot increase hydrolysis rate, but the combination of advection and diffusion increases hydrolysis rate.

Keywords. Enzymatic hydrolysis; Advection; Diffusion; Population balance equations

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